Ethyl hexanoate

123-66-0 | DTXSID3021980

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 170 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 9.42e-01

Nearest Neighbors from the Training Set

Image not found

Methyl heptanoate
Measured: 174
Predicted: 169

Image not found

Ethyl hexanoate
Measured: 167
Predicted: 170

Image not found

Propyl valerate
Measured: 168
Predicted: 169

Image not found

Hexyl acetate
Measured: 172
Predicted: 169

Image not found

Pentyl propionate
Measured: 169
Predicted: 169